A Q-operator for the quantum transfer matrix

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Abstract: Baxter's Q-operator for the quantum transfer matrix of the XXZ spin-chain is constructed employing the representation theory of quantum groups. The spectrum of this Q-operator is discussed and novel functional relations which describe the finite temperature regime of the XXZ spin-chain are derived. For non-vanishing magnetic field the previously known Bethe ansatz equations can be replaced by a system of quadratic equations which is an important advantage for numerical studies. For vanishing magnetic field and rational coupling values it is argued that the quantum transfer matrix exhibits a loop algebra symmetry closely related to the one of the classical six-vertex transfer matrix at roots of unity.

1. Introduction

In this work we present new identities for the description of the spectrum of the quantum transfer matrix for the XXZ spin-chain with non-vanishing external magnetic field h,

$$H_{\rm XXZ}=\frac{1}{2}\sum_{\ell=1}^{L}\left\{\sigma_\ell^x\sigma_{\ell+1}^x+\sigma_\ell^y\sigma_{\ell+1}^y+\Delta(\sigma_\ell^z\sigma_{\ell+1}^z-1)\right\}-\frac{h}{2}\sum_{\ell=1}^{L}\sigma^z\;. \tag{1.1}$$

Here $\Delta=(q+q^{-1})/2$ is an anisotropy parameter which is assumed to be real. This spin-chain serves as a prototype model for other more complicated integrable systems. It is an important toy model for the exact computation of physical quantities such as magnetic, electric or thermal conductivities. In this context the study of the finite temperature behaviour of the spin-chain is of crucial importance. One method to achieve this is the so-called quantum transfer matrix (see e.g. [1]),

$$\tau(z;w)=\operatorname*{Tr}_0 q^{\alpha\ \sigma^z\otimes 1}R_{0N}(zw)R^{t\otimes 1}_{(N-1)0}(w/z)\cdots R_{02}(zw)R^{t\otimes 1}_{10}(w/z),\quad q^\alpha:=e^{\beta h/2} \tag{1.2}$$

in terms of which the partition function of the XXZ spin-chain can be expressed

$$Z_L=\operatorname*{Tr}_{(\mathbb{C}^2)^{\otimes L}}e^{-\beta H_{\rm XXZ}}=\lim_{N\to\infty}\operatorname*{Tr}_{(\mathbb{C}^2)^{\otimes N}}\tau(z=1;w=e^{-\beta'/N})^L,\qquad \beta'=\beta(q-q^{-1})\;. \tag{1.3}$$

Let us explain the various objects appearing in the definition. The variable $\beta > 0$ denotes the inverse temperature of the system and for convenience we have introduced a "twist angle" $\alpha = \beta h/2\ln q$ with h being the magnetic field in (1.1). The quantum transfer matrix is built out of the well-known six-vertex R-matrix which acts on the tensor product $\mathbb{C}^2 \otimes \mathbb{C}^2$,

$$R = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \otimes \sigma^+\sigma^- + \begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix} \otimes \sigma^-\sigma^+ + c\,\sigma^+ \otimes \sigma^- + c'\,\sigma^- \otimes \sigma^+ \ . \tag{1.4}$$

Here the parametrization of the Boltzmann weights a, b, c, c' is chosen as follows[1]

$$a = 1, \quad b = \frac{(1-z)q}{1-zq^2}, \quad c = \frac{1-q^2}{1-zq^2}, \quad c' = c\,z \ . \tag{1.5}$$

The upper index $t\otimes 1$ in (1.2) stands for transposition in the first factor. We recall that the six-vertex R-matrix gives rise to a classical statistical mechanics system which is described by the *classical* six-vertex transfer matrix (as opposed to *quantum*),

$$t_{6\text{v}}(z) = \operatorname*{Tr}_0 R_{0L}(z) \cdots R_{01}(z) \ . \tag{1.6}$$

This classical physical system is connected with the above quantum spin-chain through the relation (we set temporarily $h = 0$)

$$H_{\text{XXZ}} = (q - q^{-1}) \ \ z\frac{d}{dz} \ln t_{6\text{v}}(z)\Big|_{z=1} \ . \tag{1.7}$$

The prefactor in the last equation explains the introduction of the renormalised temperature variable β' in (1.3). As an immediate consequence of (1.7) one has the following identity for the density matrix

$$\lim_{N\to\infty} \Big(t_{6\text{v}}(1)^{-1} t_{6\text{v}}(e^{-\beta'/N}) \Big)^N = e^{-\beta H_{\text{XXZ}}} \ . \tag{1.8}$$

This rewriting is inspired by the Trotter formula in the path-integral formalism of quantum field theory and N is referred to as Trotter number [4]. The last expression (1.8) can be conveniently expressed in terms of the quantum transfer matrix (1.2); see the review [2] and references therein for details. Note in particular that for this construction to work the Trotter number N has to be even and we shall work throughout this paper with the convention

$$N = 2n \ . \tag{1.9}$$

In the thermodynamic limit when the physical system size L tends to infinity the partition function (1.3) can be approximated by the largest eigenvalue Λ_N of the quantum transfer matrix (1.2),

$$L \gg 1 : \ Z_L = \lim_{N\to\infty} \operatorname*{Tr}_{(\mathbb{C}^2)^{\otimes N}} \tau(1; e^{-\beta'/N})^L \approx \lim_{N\to\infty} (\Lambda_N)^L \ . \tag{1.10}$$

[1] Below we will compare the results in this paper with the known properties about the quantum transfer matrix as they can be found in e.g. [2]. To this end it is helpful to identify the definition of the Boltzmann weights in [2] on page 11, equation (2) with ours by setting $z = e^{i\gamma w}$ and $q = e^{i\gamma}$. Note that on page 16 in [2] a rotation in the complex plane is performed replacing $w \to iv$; see equations (23) and (24) therein.

Thus, the introduction of the quantum transfer matrix (1.2) allows one to efficiently investigate the finite temperature regime. Instead of having to compute multiple excited states and energies of the quantum spin-chain (1.1) at finite temperature, one only needs to compute a single eigenvalue and eigenstate of the quantum transfer matrix (1.2). Similar simplifications occur also in the computation of finite temperature correlation functions; see for instance [3].

There are some technical complications, however. We refer the reader for the following statements to [2] and references therein. The algebraic properties of the quantum transfer matrix resemble closely the ones of the classical six-vertex transfer matrix (1.6) and as a result one can compute the eigenstates and eigenvalues of the quantum transfer matrix by similar methods as in the classical case, i.e. the algebraic Bethe ansatz. Via this route one obtains expressions for the eigenvalues of (1.2). In particular the largest eigenvalue Λ_N can be cast into the form

$$\Lambda_N(u)=\frac{e^{\frac{\beta h}{2}}\phi(u-i)\mathcal{Q}(u+2i)+e^{-\frac{\beta h}{2}}\phi(u+i)\mathcal{Q}(u-2i)}{\mathcal{Q}(u)[\sinh\frac{\gamma}{2}(u-2i+i\tau)\sinh\frac{\gamma}{2}(u+2i-i\tau)]^{\frac{N}{2}}}\ , \tag{1.11}$$

where we have set $z=e^{\gamma u},\ w=e^{-\beta'/N}=e^{-i\gamma\tau},\ q=e^{i\gamma}$ and introduced the functions

$$\phi(u)=[\sinh\tfrac{\gamma}{2}(u-i+i\tau)\sinh\tfrac{\gamma}{2}(u-2i+i\tau)]^n,\qquad \mathcal{Q}(u)=\prod_{j=1}^{n}\sinh\tfrac{\gamma}{2}(u-u_j)\ . \tag{1.12}$$

The quantities u_j are solutions of the following system of non-linear equations

$$\frac{\phi(u_j+i)}{\phi(u_j-i)}=-e^{\beta h}\frac{\mathcal{Q}(u_j+2i)}{\mathcal{Q}(u_j-2i)},\qquad j=1,...,n\ . \tag{1.13}$$

Compare with equations (25-30) in [2]. The analytic solutions to the last set of equations, known as Bethe ansatz equations, are not known. Furthermore, in the Trotter limit $N\to\infty$ the distribution of the Bethe roots u_j remains discrete and cannot be approximated by continuous density functions as it is the case for the classical transfer matrix (1.6). Instead one has to rely on the numerical solution of a non-linear integral equation. The derivation of this integral equation as well as other properties of the quantum transfer matrix are based on numerical studies of the above Bethe ansatz equations (1.13).

With this in mind it is worthwhile to study alternative methods of deriving the spectrum, and in particular the largest eigenvalue, which lead to systems of equations simpler than the Bethe ansatz equations (1.13). The purpose of this article is to diagonalise the quantum transfer matrix employing Baxter's idea of an auxiliary matrix known as Q-operator [5]. The eigenvalues of the Q-operator give the Q-function in (1.12) and we will derive a set of functional relations analogous to the ones first obtained in the context of conformal field theory [6]. The case of the finite XXZ spin-chain has been investigated in [7] and [8, 9, 10]. In particular, we will follow closely the treatment for the twisted XXZ spin-chain given in [10].

In order to construct the Q-operator we will use the representation theory of quantum groups. The main results for $h\neq 0$ in (1.1) are novel identities for the spectrum of

the quantum transfer matrix and a simpler set of equations which imply the Bethe ansatz equations (1.13) but are *quadratic* instead of order N. One of the main results in this paper is that the largest eigenvalue Λ_N of (1.2) can be expressed in terms of one polynomial

$$Q^+(z)=\sum_{k=0}^{n} e_k^+(-z)^k, \tag{1.14}$$

whose coefficients e_k^+ (with $e_0^+=1$) solve the following system of *quadratic* equations

$$e_n^+\sum_{k+l=m}\binom{n}{k}\binom{n}{l}(wq)^{k-l}=\sum_{k+l=m}\frac{\sinh[\frac{\beta h}{2}-i\gamma(k-l)]}{\sinh[\beta h/2]}\,e_k^+e_{n-l}^+\;. \tag{1.15}$$

Here the summation convention in (1.15) is to be understood as follows. First fix the variable m in the allowed range $m=1,...,N-1$ and then sum in (1.15) over all possible values for k,l such that $k+l=m$. Thus, one obtains in total $N-1$ coupled quadratic equations. For real z the largest eigenvalue of the quantum transfer matrix is then given by

$$\Lambda_N(z;w)=\frac{e^{\beta h}Q^+(zq^{-2})Q^-(zq^2)-e^{-\beta h}Q^+(zq^2)Q^-(zq^{-2})}{\sinh[\beta h/2][(zwq-1)(z/wq-1)]^{N/2}}\;, \tag{1.16}$$

where Q^- is the reciprocal polynomial of Q^+, i.e.

$$Q^-(z)=\sum_{k=0}^{n}\frac{e_{n-k}^+}{e_n^+}(-z)^k=z^nQ^+(z^{-1})/e_n^+\;.$$

In the critical regime, $q\in\mathbb{S}^1$, the coefficients e_k^+ obey the additional constraint

$$(e_k^+)^*=e_{n-k}^+/e_n^+\;. \tag{1.17}$$

There are in general many solutions to the equations (1.15) (similar as there are multiple solutions to the Bethe ansatz equations) describing a subset of the spectrum of (1.2). The largest eigenvalue of the quantum transfer matrix Λ_N appears to be always among them; this has been numerically verified for $N=2,4,6,8,10,12,14,16$ [2] and for all of these cases the total number of solutions to (1.15) is found to be 2^n.

The identities (1.15) and (1.16) are special cases of more generally valid expressions for the spectrum of the quantum transfer matrix; see equations (4.2) and (4.3) in the text. We discuss these identities in the context of higher spin quantum transfer matrices and the associated fusion hierarchy. This is motivated by the definition of a trace functional which might be relevant for the computation of correlation functions. Underlying the derivation of the main result is a concrete operator construction for $Q^\pm$ which is important to extract further information on the spectrum and also applies to the case of vanishing magnetic field, $h=0$ in (1.1), albeit one has then to restrict the deformation parameter q to a root

[2]It appears that there is a difference between $n=N/2$ odd and even; compare with the footnote in [3], Section 2.6. For n odd the largest eigenvalue might have less than n Bethe roots. Nevertheless, in the cases $N=2,6,10$ we have numercially verified that (1.15) and (1.16) still hold true.

of unity, $q^\ell = 1,\ \ell > 2$. In this case, we argue that the quantum transfer matrix exhibits a loop algebra symmetry just as the classical six-vertex transfer matrix [12] albeit in a different representation.

The outline of the article is as follows. In Section 2 we connect the structure of the quantum transfer matrix to the representation theory of the quantum affine algebra $U_q(\widehat{sl}_2)$. In particular, we discuss a specific dual representation and the corresponding L-operator. This will yield the commutation relations between the quantum monodromy matrix elements corresponding to (1.2) and the Chevalley-Serre generators of $U_q(\widehat{sl}_2)$ which allows us to prove the loop algebra symmetry $U(\tilde{sl}_2)$ of the quantum transfer matrix at roots of unity and for vanishing magnetic field. As a preparatory step for the discussion of the Q-operator we introduce the quantum fusion hierarchy, i.e. the higher spin analogues of the quantum transfer matrix.

In Section 3 we construct the Q-operator for the quantum transfer matrix and discuss its properties and functional relations. The proofs can be found in appendices A and B. For the construction of the Q-operator one has carefully to distinguish between the case of generic q and q a root of unity. In the former case the auxiliary space of the Q-operator is infinite-dimensional and one needs to introduce a boundary parameter (the external magnetic field h) in order to ensure convergence. At a root of unity the auxiliary space is finite-dimensional and the construction of Q then also applies to the case $h = 0$. However, some of the functional relations which hold true at $h \neq 0$ then cease to be valid.

Section 4 is devoted to a special Q-operator functional equation, the Wronskian relation, which suffices to compute the spectrum of the quantum transfer matrix and implies the Bethe ansatz equations. At the end we discuss some special solutions which contain the largest eigenvalue and are based on numerical evidence.

Section 5 contains the conclusions.

2. The Quantum transfer matrix and representation theory

As a preparatory step for the construction of the Q-operator for the quantum transfer matrix let us first analyse the definition (1.2) from a representation theoretic point of view. This will enable us to define the corresponding L-operator from which the Q-operator will be built.

Recall that the six-vertex R-matrix is an intertwiner of the quantum affine algebra $U_q(\widehat{sl}_2)$ with respect to the tensor product of the two-dimensional evaluation representation. The quantum affine algebra $U_q(\widehat{sl}_2)$ is generated from the Chevalley-Serre elements subject to the relations

$$q^{h_i}q^{h_j} = q^{h_j}q^{h_i}, \quad q^{h_i}e_jq^{-h_i} = q^{A_{ij}}e_j, \quad q^{h_i}f_jq^{-h_i} = q^{-A_{ij}}f_j, \quad [e_i, f_j] = \delta_{ij}\frac{q^{h_i} - q^{-h_i}}{q - q^{-1}} \tag{2.1}$$

and

$$x_i^3x_j - [3]_q x_i^2x_jx_i + [3]_q x_ix_jx_i^2 - x_jx_i^3 = 0, \quad x = e, f\ . \tag{2.2}$$

Here the indices i, j take the values 0,1 and A_{ij} is the Cartan matrix of $\widehat{sl}_2$. The evaluation homomorphism $ev_z : U_q(\widehat{sl}_2) \to U_q(sl_2)$ defined by

$$ev_z(e_0) = z\ f, \quad ev(f_0) = z^{-1}e, \quad ev(q^{h_0}) = q^{-h} \tag{2.3}$$

and

$$ev(e_1) = e, \quad ev(f_1) = f, \quad ev(q^{h_1}) = q^h\ . \tag{2.4}$$

An evaluation representation is now obtained by combining the evaluation homomorphism with any finite-dimensional representation of $U_q(sl_2)$, in particular we can choose the two-dimensional, spin 1/2 representation in terms of Pauli matrices,

$$\pi(e) = \sigma^+, \quad \pi(f) = \sigma^-, \quad \pi(q^h) = q^{\sigma^z}\ . \tag{2.5}$$

The six-vertex R-matrix then intertwines the tensor product representation $\pi_z \otimes \pi_1$ with $\pi_z = \pi \circ ev_z$.

Given any representation $\rho : U_q(\widehat{sl}_2) \to \operatorname{End} V$ over some finite-dimensional vector space V we define the following representation over its dual space V^*,

$$\rho^* : U_q(\widehat{sl}_2) \to \operatorname{End} V^*, \qquad \langle \rho^*(x)v^*, w\rangle := \left\langle v^*, \rho(\gamma^{-1}(x))w\right\rangle, \quad x \in U_q(\widehat{sl}_2),\ w \in V\ . \tag{2.6}$$

Here γ is the antipode which is defined on the Chevalley-Serre generators as follows,

$$\gamma(e_i) = -q^{-h_i}e_i, \qquad \gamma(f_i) = -f_i q^{h_i}, \qquad \gamma(q^{\pm h_i}) = q^{\mp h_i} \tag{2.7}$$
$$\gamma^{-1}(e_i) = -e_i q^{-h_i}, \qquad \gamma^{-1}(f_i) = -q^{h_i} f_i, \qquad \gamma^{-1}(q^{\pm h_i}) = q^{\mp h_i}\ . \tag{2.8}$$

If we canonically identify V^* with V the representation ρ^* in terms of matrices is simply given by

$$\rho^*(x) = (\rho(\gamma^{-1}(x)))^t, \qquad x \in U_q(\widehat{sl}_2) \tag{2.9}$$

with t denoting the transpose. Note that the definition (2.7) is compatible with the following choice for the coproduct

$$\Delta(e_i) = e_i \otimes 1 + q^{h_i} \otimes e_i, \qquad \Delta(f_i) = f_i \otimes q^{-h_i} + 1 \otimes f_i, \qquad \Delta(q^{h_i}) = q^{h_i} \otimes q^{h_i}\ . \tag{2.10}$$

Setting $\rho = \pi$, the two-dimensional evaluation module, we are interested in finding the intertwiner

$$L^*\ \Delta^*(x) = \Delta^*_{\mathrm{op}}(x) L^* \quad \text{with} \quad \Delta^* = (1 \otimes \pi^*)\Delta \quad \text{and} \quad L^* \in U_q(sl_2) \otimes \operatorname{End} V^*\ . \tag{2.11}$$

Explicitly, the coproduct relations for the Chevalley-Serre generators read

$$\Delta^*(e_1) = e_1 \otimes 1 - q^{1+h_1} \otimes \sigma^-, \qquad \Delta^*_{\mathrm{op}}(e_1) = e_1 \otimes q^{-\sigma^z} - q\ 1 \otimes \sigma^-\ , \tag{2.12}$$
$$\Delta^*(f_1) = f_1 \otimes q^{\sigma^z} - q^{-1} 1 \otimes \sigma^+, \qquad \Delta^*_{\mathrm{op}}(f_1) = f_1 \otimes 1 - q^{-1-h_1} \otimes \sigma^+\ , \tag{2.13}$$

and

$$\pi^*(e_1) = -(\sigma^+ q^{-\sigma^z})^t = -q\ \sigma^-, \qquad \pi^*(f_1) = -(q^{\sigma^z}\sigma^-)^t = -q^{-1}\sigma^+, \tag{2.14}$$
$$\pi^*(e_0) = -(\sigma^- q^{\sigma^z})^t = -q\ \sigma^+, \qquad \pi^*(f_0) = -(q^{-\sigma^z}\sigma^+)^t = -q^{-1}\sigma^-\ . \tag{2.15}$$

We will see below that the intertwiner (2.11) specializes to the R-matrix used in the definition of the quantum transfer matrix (1.2). Solving the above intertwining condition (2.11) for an evaluation module with central charge zero, i.e. $q^{h_0} = q^{-h_1}$, we find

$$L^*(z) = \begin{pmatrix} zq^{-\frac{h_1+1}{2}} - q^{\frac{h_1+1}{2}} & (q^{-1}-q)e_1 q^{-\frac{h_1+1}{2}} \\ z(q^{-1}-q)q^{\frac{h_1+1}{2}} f_1 & zq^{\frac{h_1-1}{2}} - q^{-\frac{h_1-1}{2}} \end{pmatrix} . \tag{2.16}$$

For comparison and in order to keep this article self-contained recall that the conventional L-operator reads

$$L(z) = \begin{pmatrix} zq^{\frac{h_1+1}{2}} - q^{-\frac{h_1+1}{2}} & z(q-q^{-1})q^{\frac{h_1+1}{2}} f_1 \\ (q-q^{-1})e_1 q^{-\frac{h_1+1}{2}} & zq^{-\frac{h_1-1}{2}} - q^{\frac{h_1-1}{2}} \end{pmatrix} . \tag{2.17}$$

In light of the following identity for the universal R-matrix $(1 \otimes \gamma^{-1})\boldsymbol{R} = \boldsymbol{R}^{-1}$ it would be more natural to use $-z^{-1}L^*(z)$ as intertwiner for the dual representation π^*. However, we wish for later purposes to keep the L^*-operator polynomial in z instead of z^{-1}. Evaluating this intertwiner in the two-dimensional spin 1/2 representation (2.5) yields

$$R^{\pi,\pi^*}(z) = \frac{(\pi \otimes 1)L^*(z)}{zq^{-1} - q} = \left(R(z)^{-1}\right)^{1\otimes t} = [R_{21}(z^{-1})]^{1\otimes t} , \tag{2.18}$$

which is one of the R-matrices used in the definition of the quantum transfer matrix (1.2). Thus, we conclude that one lattice row associated with the monodromy matrix of the quantum transfer matrix corresponds to the following quantum group module

$$\pi_z \otimes \mathfrak{M}_w^{(N)}, \qquad \mathfrak{M}_w^{(N)} = \underbrace{\pi_w^* \otimes \pi_{w^{-1}} \cdots \otimes \pi_w^* \otimes \pi_{w^{-1}}}_{N} . \tag{2.19}$$

From this we immediately deduce that the quantum transfer matrix $\tau(z; w)$ block decomposes with respect to the following alternating spin operator,

$$[\tau(z; w), S_A] = 0, \qquad S_A := \frac{1}{2}\sum_{k=1}^{N} (-)^k \sigma_k^z , \tag{2.20}$$

since the quantum monodromy matrix

$$R_{0N}(zw)R^{t\otimes 1}_{(N-1)0}(w/z) \cdots R_{02}(zw)R^{t\otimes 1}_{10}(w/z) = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z) \end{pmatrix} \tag{2.21}$$

is an intertwiner with respect to the tensor product (2.19). More generally, we have

$$[A, q^{H_1}] = [D, q^{H_1}] = 0,\ q^{H_1} B q^{-H_1} = q^{-2}B,\ q^{H_1} C q^{-H_1} = q^2 C, \qquad q^{H_1} = q^{2S_A} . \tag{2.22}$$

Denoting the Chevalley-Serre generators acting in quantum space (2.19) by capital letters, $\{E_1, E_0, F_1, F_0, H_0 = -H_1\}$, one finds the analogous commutation relations as in the classical case; see equations (14-15) in [13]. The difference between the relations for the classical and the quantum transfer matrix is purely in the explicit form of the quantum

group generators which is fixed through the identification of the quantum group module $\mathfrak{M}_w^{(N)}$ in (2.19). For instance, employing (2.10) and (2.5), (2.14) one has

$$E_1 = \sum_{k=1}^{N} \varepsilon_k q^{\frac{1-\varepsilon_k}{2}} \left(\prod_{j<k} q^{\varepsilon_j \sigma_j^z} \right) \sigma_k^{\varepsilon_k}, \qquad \varepsilon_k = (-1)^k \tag{2.23}$$

$$F_1 = \sum_{k=1}^{N} \varepsilon_k q^{\frac{\varepsilon_k - 1}{2}} \sigma_k^{-\varepsilon_k} \left(\prod_{j>k} q^{-\varepsilon_j \sigma_j^z} \right), \tag{2.24}$$

and so forth. Following the same line of argument as presented in [13] (c.f. equations (23-24) therein) one then proves that for zero magnetic field $h = 0$ and q being a primitive root of unity of order ℓ the quantum transfer matrix (1.2) enjoys a loop algebra symmetry $U(\widetilde{sl}_2)$ in the sectors

$$2S_A = 0 \bmod \ell \; . \tag{2.25}$$

The Chevalley-Serre generators of the loop algebra $U(\widetilde{sl}_2)$ are obtained from the restricted quantum group (compare with the discussion in [14]) via taking the following limit from generic q' to the root of unity value q,

$$q^\ell = 1 : \qquad E_1^{(\ell')} := \lim_{q' \to q} E_1^{\ell'} / [\ell']_{q'}!, \qquad [x]_q := \frac{q^x - q^{-x}}{q - q^{-1}}, \quad \ell' = \begin{cases} \ell, & \text{if } \ell \text{ is odd} \\ \ell/2, & \text{if } \ell \text{ is even} \end{cases} .$$

Analogous expressions hold for the remaining generators. All of the Chevalley-Serre generators, $\{E_1^{(\ell')}, E_0^{(\ell')}, F_1^{(\ell')}, F_0^{(\ell')}\}$, commute in the commensurate sectors (2.25) with the quantum transfer matrix, e.g.

$$[\tau(z; w), E_1^{(\ell')}] = 0 \qquad \text{for } \; h = 0, \quad q^\ell = 1 \quad \text{and} \quad 2S_A = 0 \bmod \ell \; . \tag{2.26}$$

This result for the quantum transfer matrix is analogous to the loop symmetry of the classical transfer matrix first discovered in [12], albeit via a different proof.

2.1 Transformation under spin reversal

In order to show the existence of two independent solutions to the TQ-equation, we discuss the behaviour of the quantum transfer matrix under spin-reversal. From the elementary identities

$$\begin{aligned} (1 \otimes \sigma^x) R(z) (1 \otimes \sigma^x) &= (\sigma^x \otimes z^{-\frac{\sigma^z}{2}}) R(z) (\sigma^x \otimes z^{\frac{\sigma^z}{2}}) \\ (1 \otimes \sigma^x) R^*(z) (1 \otimes \sigma^x) &= (\sigma^x \otimes z^{\frac{\sigma^z}{2}}) R^*(z) (\sigma^x \otimes z^{-\frac{\sigma^z}{2}}) \end{aligned}$$

we infer that the quantum transfer matrix (1.2) transforms as

$$w^{S^z} \mathfrak{R} \; \tau_\alpha(z; w) \; w^{S^z} \mathfrak{R} = \tau_{-\alpha}(z; w) \tag{2.27}$$

under the involution $w^{S^z} \mathfrak{R}$ with

$$\mathfrak{R} = \prod_{j=1}^{N} \sigma_j^x \qquad \text{and} \qquad S^z = \frac{1}{2} \sum_{j=1}^{N} \sigma_j^z \; . \tag{2.28}$$

In addition, the quantum transfer matrix obeys another identity. First we observe that the following equations for the Boltzmann weights (1.5) hold true,

$$a_{z^{-1}}=1,\quad b_{z^{-1}}=1/b_{zq^{-2}},\quad c_{z^{-1}}=-q\,c'_{zq^{-2}}/b_{zq^{-2}},\quad c'_{z^{-1}}=-q^{-1}c_{zq^{-2}}/b_{zq^{-2}}\,. \tag{2.29}$$

Employing the identities

$$\begin{aligned}R(z^{-1}) &= \frac{1}{b_{zq^{-2}}}\,(\sigma^x\otimes(-q)^{-\frac{\sigma^z}{2}})R(zq^{-2})^{1\otimes t}(\sigma^x\otimes(-q)^{\frac{\sigma^z}{2}})\\ R^*(z^{-1}) &= \frac{1}{b_{z^{-1}q^{-2}}}\,(\sigma^x\otimes(-q)^{\frac{\sigma^z}{2}})R^*(zq^2)^{1\otimes t}(\sigma^x\otimes(-q)^{-\frac{\sigma^z}{2}})\end{aligned}$$

we then easily find the expression for the transpose of the quantum transfer matrix,

$$\begin{aligned}\tau_{-\alpha}(z^{-1},w^{-1}) &= \operatorname*{Tr}_0 q^{-\alpha\ \sigma^z\otimes 1}R_{0N}(z^{-1}w^{-1})R^*_{0N-1}(w/z)\cdots R_{02}(z^{-1}w^{-1})R^*_{01}(w/z)\\ &= \frac{\tau_\alpha(z,wq^{-2})^t}{b^n_{zwq^{-2}}b^n_{wq^{-2}/z}},\end{aligned} \tag{2.30}$$

where we have used that $[S_A,\tau_\alpha(z,w)]=0$.

2.2 The quantum fusion hierarchy

The quantum transfer matrix (1.2) commutes with an infinite family of higher spin transfer matrices. In close analogy with the classical six-vertex model we define for $d\in\mathbb{N}$ the following family of transfer matrices,[3]

$$\tau^{(d-1)}(z;w)=\operatorname*{Tr}_{\pi^{(d-1)}} q^{\alpha h\otimes 1}L_N(zw)L^*_{N-1}(z/w)\cdots L_2(zw)L^*_1(z/w),\qquad q^\alpha=e^{\frac{h\beta}{2}}\ , \tag{2.31}$$

where the representation in auxiliary space has been replaced by the spin $(d-1)/2$ evaluation module $\pi^{(d-1)}$,

$$\pi^{(d-1)}(e)\,|k\rangle=[d{-}k]_q\,|k-1\rangle\ ,\ \pi^{(d-1)}(f)\,|k\rangle=[k{+}1]_q\,|k+1\rangle\ ,\ \pi^{(d-1)}(q^h)\,|k\rangle=q^{d-2k-1}\,|k\rangle\ , \tag{2.32}$$

where the index k labelling the basis vectors of the representation takes values in the set $k=0,1,2,...,d-1$ and we set $e\,|0\rangle=f\,|d-1\rangle=0$. Our motivation for introducing (2.31) is twofold. They are natural objects to consider from a representation theoretic point of view and we will encounter them when deriving functional relations for the Q-operator in the subsequent section. The other reason is their extension to complex dimension $d\in\mathbb{C}$ which is closely related to the trace functional used in recent formulations for correlation functions [11].

Setting $d=2$ we identify $\pi^{(1)}\equiv\pi$ in (2.5) and recover the quantum transfer matrix via the relation

$$\tau(z;w)=\frac{(-z/w)^{-n}\tau^{(1)}(z;w)}{(zwq-q^{-1})^n(wq/z-q^{-1})^n}=\frac{\tau^{(1)}(z;w)}{(zwq-q^{-1})^n(z/wq-q)^n}\ . \tag{2.33}$$

[3] In the following we shall often suppress the explicit dependence on the temperature parameter w.

The spin 0 representation yields the quantum determinant,

$$\begin{aligned}\tau^{(0)}(z;w) &= (zwq^{\frac{1}{2}} - q^{-\frac{1}{2}})^n(zq^{-\frac{1}{2}}/w - q^{\frac{1}{2}})^n \\ &= (zw - q^{-1})^n(z/w - q)^n = (zwq-1)^n(z/wq-1)^n \end{aligned} \tag{2.34}$$

Similar to the classical six-vertex model, the higher-spin quantum transfer matrices $\tau^{(d)}$ satisfy a functional relation known as the fusion hierarchy,

$$\tau^{(d-1)}(zq^d)\tau^{(1)}(z) = \tau^{(0)}(zq^{-1})\tau^{(d-2)}(zq^{d+1}) + \tau^{(0)}(zq)\tau^{(d)}(zq^{d-1}) \tag{2.35}$$

which is a corollary of the decomposition of the tensor product $\pi^{(d-1)}_{zq^d} \otimes \pi^{(1)}_z$ described by the exact sequence

$$0 \to \pi^{(d-2)}_{zq^{d+1}} \overset{\imath}{\hookrightarrow} \pi^{(d-1)}_{zq^d} \otimes \pi^{(1)}_z \xrightarrow{p} \pi^{(d)}_{zq^{d-1}} \to 0\ . \tag{2.36}$$

Since the auxiliary spaces in the quantum transfer matrices are the same as in the classical case, we can use the same representation theoretic results to derive all relevant functional relations. What changes in the transition from "classical" to "quantum" are the coefficient functions which appear in the respective functional equation. For instance, the coefficients $\tau^{(0)}(zq^{-1}),\ \tau^{(0)}(zq)$ follow from the identities

$$\begin{aligned}(\pi^{(d-1)}\otimes 1)L_{13}(zq^d)R_{23}(z)(\imath\otimes 1) &= (z-1)(\imath\otimes 1)(\pi^{(d-2)}\otimes 1)L(zq^{d+1}) \\ (p\otimes 1)(\pi^{(d-1)}\otimes 1)L_{13}(zq^d)R_{23}(z) &= \left(zq - q^{-1}\right)(\pi^{(d)}\otimes 1)L(zq^{d-1})(p\otimes 1)\end{aligned} \tag{2.37}$$

and

$$\begin{aligned}(\pi^{(d-1)}\otimes 1)L^*_{13}(zq^d)R^*_{23}(z)(\imath\otimes 1) &= (z^{-1}q - q^{-1})(\imath\otimes 1)(\pi^{(d-2)}\otimes 1)L^*(zq^{d+1}) \\ (p\otimes 1)(\pi^{(d-1)}\otimes 1)L^*_{13}(zq^d)R_{23}(z) &= (z^{-1}-1)(\pi^{(d)}\otimes 1)L^*(zq^{d-1})(p\otimes 1)\end{aligned} \tag{2.38}$$

where the maps

$$\imath:\ |k\rangle \hookrightarrow [d-k-1]_q\,|k\rangle\otimes|1\rangle - q^{d-k-1}[k+1]_q\,|k+1\rangle\otimes|0\rangle \tag{2.39}$$

and

$$p:\ \frac{[d]}{[d-k]}\ |k\rangle\otimes|0\rangle \to |k\rangle \tag{2.40}$$

are the inclusion and projection map in the exact sequence (2.36).

3. The Quantum Q-operator

After outlining the derivation of (2.35) we now turn to the Q-operator and apply the same strategy as in the case of the fusion hierarchy. The main difference lies in the fact that for the definition of the Q-operator we need to introduce an *infinite*-dimensional evaluation module when q is generic (i.e. not a root of unity) [7] [8],

$$\begin{aligned}\rho^+(e_0)\,|k\rangle &= z\,|k+1\rangle\,, \quad \rho^+(q^{\frac{h_1}{2}})\,|k\rangle = \rho^+(q^{-\frac{h_0}{2}})\,|k\rangle = r^{\frac{1}{2}}q^{-k-1/2}\,|k\rangle\,, \\ \rho^+(e_1)\,|k\rangle &= \frac{s+1-q^{2k}-sq^{-2k}}{(q-q^{-1})^2}\ |k-1\rangle\,, \quad \rho^+(e_1)\,|0\rangle = 0, \quad r,s,z\in\mathbb{C}\ .\end{aligned} \tag{3.1}$$

Here s, r are free parameters characterizing the representation and z denotes the spectral variable as before. In connection with spin-reversal one also encounters the module

$$\rho^- := \rho^+ \circ \omega \quad \text{with} \quad \{e_1, e_0, q^{\frac{h_1}{2}}, q^{\frac{h_0}{2}}\} \xrightarrow{\omega} \{e_0, e_1, q^{\frac{h_0}{2}}, q^{\frac{h_1}{2}}\} \,. \tag{3.2}$$

Note that in the limit $s \to 0$ we recover the q-oscillator representations used in [6]. In the case that q is a primitive root of unity of order ℓ we truncate the evaluation module ρ^+ by imposing the condition (compare with [9])

$$q^\ell = 1: \qquad \rho^+(e_0)\left|\ell' - 1\right\rangle = 0, \quad \ell' = \begin{cases} \ell, & \text{if } \ell \text{ is odd} \\ \ell/2, & \text{if } \ell \text{ is even} \end{cases} \,. \tag{3.3}$$

The intertwiner corresponding to the quantum group module $\rho^+ \otimes \pi$ has been computed previously [7] [8] and reads,

$$\mathfrak{L}(z) = \begin{pmatrix} z\frac{s}{r}\; q^{\frac{h_1+1}{2}} - q^{-\frac{h_1+1}{2}} & (q - q^{-1})q^{\frac{h_1+1}{2}} e_0 \\ (q - q^{-1}) e_1 q^{-\frac{h_1+1}{2}} & zr\; q^{-\frac{h_1-1}{2}} - q^{\frac{h_1-1}{2}} \end{pmatrix} \in U_q(\widehat{sl}_2) \otimes \operatorname{End} V \,. \tag{3.4}$$

In order to define a Q-operator for the quantum transfer matrix we now need to compute the intertwiner corresponding to the module $\rho^+ \otimes \pi^*$. The result is

$$\mathfrak{L}^*(z) = \begin{pmatrix} zr\; q^{-\frac{h_1+1}{2}} - q^{\frac{h_1+1}{2}} & (q^{-1} - q) e_1 q^{-\frac{h_1+1}{2}} \\ (q^{-1} - q) q^{\frac{h_1+1}{2}} e_0 & z\frac{s}{r}\; q^{\frac{h_1-1}{2}} - q^{-\frac{h_1-1}{2}} \end{pmatrix} \in U_q(\widehat{sl}_2) \otimes \operatorname{End} V^* \,. \tag{3.5}$$

The last expression is derived from the coproduct relations

$$\begin{aligned} \Delta^*(e_1) &= e_1 \otimes 1 - q^{1+h_1} \otimes \sigma^-, \qquad & \Delta^*_{\text{op}}(e_1) &= e_1 \otimes q^{-\sigma^z} - q\; 1 \otimes \sigma^-, \\ \Delta^*(e_0) &= e_0 \otimes 1 - q^{1+h_0} \otimes \sigma^+, \qquad & \Delta^*_{\text{op}}(e_0) &= e_0 \otimes q^{\sigma^z} - q\; 1 \otimes \sigma^+ \,. \end{aligned} \tag{3.6}$$

We define for $r = 1$ in ρ^+ the operator

$$Q(z; s) = \operatorname*{Tr}_{\rho^+} q^{\alpha h_1 \otimes 1} \mathfrak{L}_N(zw) \mathfrak{L}^*_{N-1}(z/w) \cdots \mathfrak{L}_2(zw) \mathfrak{L}^*_1(z/w), \quad q^\alpha = e^{\beta h/2}, \tag{3.7}$$

where we have normalised (3.5) such that Q is polynomial in the spectral parameter z. The specialization to $r = 1$ can be imposed without any loss loss of generality due to the identity

$$Q(z; r, s) = r^{\alpha - S_A} Q(z; r = 1, s) \,. \tag{3.8}$$

Having stated the explicit definition of the Q-operator we now turn to its properties and the functional relations it satisfies. Since the auxiliary spaces of the quantum transfer matrix and the Q-operator are the same as in the conventional, classical six-vertex model the proofs for the statements made below follow closely the line of argument presented previously in [8, 9, 10]. I shall therefore omit the proofs from the main text and refer the reader to the appendix for further details.

3.1 Factorisation

One important result is that the Q-operator factorises into simpler operators as follows (we still assume $\alpha \neq 0$),

$$Q(z;s) = Q(0;s)Q^+(z)Q^-(zs), \tag{3.9}$$

where

$$Q^+(z) = \lim_{s\to 0} Q(0;s)^{-1}Q(z;s) \tag{3.10}$$

and the normalisation factor $Q(0;s)$ at $z=0$ is easily computed to be

$$\lim_{z\to 0} Q(z;s) = \operatorname*{Tr}_{\rho^+} q^{(\alpha-S_A)h_1} = \begin{cases} \dfrac{1}{q^{\alpha-S_A}-q^{S_A-\alpha}}, & q \text{ generic} \\ \dfrac{1-q^{2\ell(S_A-\alpha)}}{q^{\alpha-S_A}-q^{S_A-\alpha}}, & q^\ell = \pm 1 \end{cases} . \tag{3.11}$$

The identity (3.11) for generic q has to be understood as analytic continuation from the region of convergence. Note that the point $\alpha = 0$, i.e. vanishing magnetic field $h = 0$, remains singular. This can be understood from the construction of the Q-operator since for generic q the auxiliary space given by the the representation (3.1) is infinite-dimensional and twisted boundary conditions with an appropriate choice of α are needed to ensure that the trace in (3.7) is well-defined; compare with the discussion in [8]. The remaining operator Q^- is the counterpart of Q^+ and can be obtained by employing the following transformation,

$$Q(z^{-1},w^{-1};s) = z^{-N}s^{\frac{N}{2}+S_A}\,(w/q)^{-S^z}\mathfrak{R}\,Q(z/s,wq^{-2};s)^t\,\mathfrak{R}(w/q)^{S^z} . \tag{3.12}$$

Here the operators $S^z, \mathfrak{R}$ have been introduced earlier in (2.28) and use has been made of the identities

$$\begin{aligned} \mathfrak{L}(z^{-1}) &= -z^{-1}q(1\otimes(-\tfrac{z}{sq})^{-\sigma^z}\sigma^x)\mathfrak{L}(zq^{-2}/s)^{1\otimes t}(1\otimes\sigma^x(-\tfrac{z}{sq})^{\sigma^z})s^{\frac{1+\sigma^z}{2}} \\ \mathfrak{L}^*(z^{-1}) &= -z^{-1}q^{-1}(1\otimes(-\tfrac{zq}{s})^{\sigma^z}\sigma^x)\mathfrak{L}^*(zq^2/s)^{1\otimes t}(1\otimes\sigma^x(-\tfrac{zq}{s})^{-\sigma^z})s^{\frac{1-\sigma^z}{2}} . \end{aligned}$$

The identity (3.12) then implies that up to an unimportant normalization constant we have,

$$Q^-(z,w) \propto z^{\frac{N}{2}+S_A}\,(wq)^{S^Z}\mathfrak{R}\,Q^+(z^{-1},w^{-1}q^{-2})^t\,\mathfrak{R}(wq)^{-S^Z} . \tag{3.13}$$

Note that the action of the spin-reversal operator relates Q^- to the representation (3.2). Both operators $Q^\pm$ have polynomial eigenvalues w.r.t. the spectral variable z. I shall denote these eigenvalues by the same symbol as the operators,

$$Q^\pm(z) = \prod_{k=1}^{n_\pm}(1-x_k^\pm z) = \sum_{k=0}^{n_\pm} e_k^\pm(-z)^k, \qquad n_\pm = n \mp S_A . \tag{3.14}$$

As we will see below the polynomial roots $x_k^\pm$ are two sets of Bethe roots. They can be (numerically) computed by employing a number of functional relations which are satisfied by the Q-operator.

3.2 Functional relations

The best known functional relation is the generalization of Baxter's TQ-equation for the six-vertex model. This equation is obtained in the present construction for the Q-operator (which differs from Baxter's approach) by first deriving the functional relation

$$Q(z;s)\tau^{(1)}(z) = q^{\alpha-S_A}\tau^{(0)}(zq)Q(zq^{-2};sq^2) + q^{S_A-\alpha}\tau^{(0)}(zq^{-1})Q(zq^2;sq^{-2}) \tag{3.15}$$

which is a direct consequence of the following decomposition of the tensor product of representations, $\rho^+(z;r,s)\otimes\pi_z$, described by the exact sequence [7] [8]

$$0 \to \rho^+(zq^2;rq^{-1},sq^{-2}) \hookrightarrow \rho^+(z;r,s)\otimes\pi_z \to \rho^+(zq^{-2},rq,sq^2) \to 0\ . \tag{3.16}$$

Here $\tau^{(0)}$ is the quantum determinant introduced in (2.34). Taking the limit $s\to 0$ employing (3.10) we obtain the TQ-equation,

$$Q^+(z)\tau^{(1)}(z) = q^{\alpha-S_A}\tau^{(0)}(zq)Q^+(zq^{-2}) + q^{S_A-\alpha}\tau^{(0)}(zq^{-1})Q^+(zq^2)\ . \tag{3.17}$$

A similar relation holds for Q^- when employing the transformations (2.27), (2.30) and (3.12). The TQ equation holds true also for vanishing external magnetic field, i.e. $\alpha = 0$. If the magnetic field is nonzero, however, there is another identity which makes use of both solutions $Q^\pm$ and on which we will focus. It yields a simple expression for all elements in the fusion hierarchy in terms of $Q^\pm$,

$$\tau^{(d-1)}(z) = \frac{q^{d(\alpha-S_A)}Q^+(zq^{-d})Q^-(zq^d) - q^{d(S_A-\alpha)}Q^+(zq^d)Q^-(zq^{-d})}{q^{\alpha-S_A}-q^{S_A-\alpha}}\ . \tag{3.18}$$

The last expression can even be analytically continued to complex dimension d if one wishes to make contact with the trace functional introduced in the context of correlation functions for the infinite XXZ spin-chain. Here we shall not pursue this aspect further but refer the reader to [11] and references therein; see also [10].

4. The Wronskian relation

Note that when setting $d = 1$ in (3.18) the left hand side of the above equation is explicitly known and we arrive at

$$(zwq-1)^n(z/wq-1)^n = \frac{q^{\alpha-S_A}Q^+(zq^{-1})Q^-(zq) - q^{S_A-\alpha}Q^+(zq)Q^-(zq^{-1})}{q^{\alpha-S_A}-q^{S_A-\alpha}}\ . \tag{4.1}$$

This functional relation, which is the discrete analogue of a Wronskian in the theory of second order differential equations, can therefore be employed to compute the eigenvalues of $Q^\pm$. It is this observation which we will investigate further in the remainder of this paper.

4.1 System of quadratic equations

Expanding the Wronskian relation (4.1) with respect to the spectral parameter z yields the following system of N-quadratic equations for the unknown coefficients $e_k^\pm$ which are the elementary symmetric polynomials in the Bethe roots,

$$\sum_{k+l=m} \binom{n}{k}\binom{n}{l}(wq)^{k-l} = \sum_{k+l=m} \frac{q^{\alpha-S_A-k+l}-q^{S_A-\alpha+k-l}}{q^{\alpha-S_A}-q^{S_A-\alpha}}\; e_k^+ e_l^- \;. \tag{4.2}$$

It should be emphasized once more that this set of equations contains for $\alpha \neq 0$ all the necessary information about the spectrum of the quantum transfer matrix as well as the higher spin transfer matrices. Recall that N is the Trotter number, $w = e^{-\beta'/N} = \exp(-\frac{\beta(q-q^{-1})}{N})$ contains the temperature variable and $q^\alpha = e^{h\beta/2}$ the external magnetic field. Setting now $n = 2$ in (3.18) the eigenvalues of the quantum transfer matrix (1.2) are obtained from the identity

$$\tau(z;w) = \frac{q^{2(\alpha-S_A)}Q^+(zq^{-2})Q^-(zq^2) - q^{2(S_A-\alpha)}Q^+(zq^2)Q^-(zq^{-2})}{(q^{\alpha-S_A}-q^{S_A-\alpha})(zwq-q^{-1})^n(z/wq-q)^n}\;. \tag{4.3}$$

The equations (4.2) and (4.3) are the aforementioned generalisations of the identities (1.15) and (1.16) in the introduction.

4.1.1 The Bethe ansatz equations

Having identified (4.2) as the key relation in describing the spectrum of the quantum transfer matrix for finite N we need to discuss the relation with the Bethe ansatz equations which are usually considered to be the fundamental set of identities for discussing the spectrum. Starting from the quantum Wronskian we set

$$z = q/x_i^+ : \qquad \frac{-q^{S_A-\alpha}Q^+(q^2/x_i^+)Q^-(1/x_i^+)}{q^{\alpha-S_A}-q^{S_A-\alpha}} = (wq^2/x_i^+-1)^n(1/wx_i^+-1)^n$$

$$z = q^{-1}/x_i^+ : \qquad \frac{q^{\alpha-S_A}Q^+(q^{-2}/x_i^+)Q^-(1/x_i^+)}{q^{\alpha-S_A}-q^{S_A-\alpha}} = (w/x_i^+-1)^n(q^{-2}/wx_i^+-1)^n$$

and obtain

$$-q^{-2\alpha}\prod_{j=1}^{n_+}\frac{x_j^+ q/x_i^+ - q^{-1}}{x_j^+ q^{-1}/x_i^+ - q} = \left(\frac{wq - x_i^+ q^{-1}}{q^{-1}-wx_i^+ q}\right)^n \left(\frac{1-wx_i^+}{w-x_i^+}\right)^n \;. \tag{4.4}$$

The last equation is one among the n_+ Bethe ansatz equations as they can be found for instance in [2]; see equations (29) and (30). To facilitate the comparison note that under the parametrisation

$$x_i = e^{\gamma\lambda_i}, \qquad q = e^{i\gamma}, \qquad w = e^{-i\gamma\tau} = e^{-(q-q^{-1})\beta/N}, \qquad q^{2\alpha} = e^{\beta h}$$

the Bethe ansatz equations are rewritten as

$$\frac{\phi(\lambda_j+i)}{\phi(\lambda_j-i)} := \frac{\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j-i\tau+2i)\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j+i\tau)}{\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j+i\tau-2i)\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j-i\tau)} =$$

$$-e^{\beta h}\prod_{k=1}^{n_+}\frac{\sinh\frac{\gamma}{2}(\lambda_j-\lambda_k+2i)}{\sinh\frac{\gamma}{2}(\lambda_j-\lambda_k-2i)} =: -e^{\beta h}\frac{\mathcal{Q}(\lambda_j+2i)}{\mathcal{Q}(\lambda_j-2i)}$$

which is the notation used in [2]. From this we infer that the Wronskian relation (4.1) implies the Bethe ansatz equations, the converse is not true. Note that Q^- yields another set of Bethe roots, which in terms of the algebraic Bethe ansatz (see the appendix) allow one to construct the eigenvector from the lowest (instead of the highest) weight vector.

4.2 Special solutions in the $S_A = 0$ sector

As pointed out earlier the quantum transfer matrix block decomposes with respect to the alternating spin-operator S_A. In particular, the largest eigenvalue Λ_N appears to be in the $S_A = 0$ sector. Since $\lim_{N\to\infty} \Lambda_N$ yields the partition function (1.3) in the thermodynamic limit its corresponding solutions to (4.2) are of particular, physical interest.

Quite generally, we infer from (4.1) that there are certain symmetries among the solutions to the Wronskian relation, for instance when replacing $z \to z^{-1}$. It is then natural to assume that some solutions are invariant under these transformations, especially when they belong to non-degenerate or distinguished eigenvalues such as Λ_N. Thus, one would expect that there is a subset of solutions for which

$$Q^{\pm}(z) = \prod_{i=1}^{n} (1 - z/x_i^{\mp}) \tag{4.5}$$

holds. That is, $Q^{\pm}$ are the inverse or reciprocal polynomial of each other. In fact, one verifies numerically for Trotter numbers up to 16 that in the $S_A = 0$ sector there are always 2^n such "special" solutions (for q real or on the unit circle) and that among this set of solutions is the one describing the largest eigenvalue of the quantum transfer matrix. Conjecturing this to be true for all N one can then halve the number of variables in (4.2) arriving at the result (1.15), (1.16) stated in the introduction. A similar observation has been made previously for the twisted XXX spin-chain; see Section 5.1 in [15].

Provided that q (and therefore $w = \exp[(q - q^{-1})\beta/N]$) lies on the unit circle there is another obvious "symmetry" of (4.1), complex conjugation. In fact, one finds for $S_A = 0$ that there exist solutions $Q^{\pm}$ invariant under this transformation, i.e. obeying the additional restriction

$$Q^{\pm}(z) = \prod_{i=1}^{n} (1 - (x_i^{\mp})^* z), \quad z \in \mathbb{R}\,. \tag{4.6}$$

In terms of the elementary symmetric polynomials $e_k^{\pm}$ the restrictions (4.5) and (4.6) correspond to the identities

$$e_k^{\pm} = e_{n-k}^{\mp}/e_n^{\mp} \qquad \text{and} \qquad e_k^{\pm} = (e_k^{\mp})^*, \tag{4.7}$$

respectively. Whether these solutions persist for Trotter numbers $N > 16$ needs to be investigated numerically. We leave this to future work.

5. Conclusions and outlook

In this paper Baxter's Q-operator has been constructed for the quantum transfer matrix of the XXZ spin-chain. The main motivation has been to derive a set of equations which

allow one to describe the spectrum of the quantum transfer matrix and are simpler than the previously known Bethe ansatz equations. For non-vanishing external magnetic field this is indeed possible and the order of the equations can be reduced from N (Bethe ansatz equations (4.4)) to order two (the Wronskian relation (4.2)) which is a great simplification for numerical computations. Of particular interest is the largest eigenvalue of the quantum transfer matrix which in the thermodynamic limit (i.e. the physical system size L tends to infinity) contains all the relevant finite temperature behaviour of the spin-chain. For this eigenvalue we observed further simplifications in its polynomial structure which lead to a reduction of the number of variables by a factor two. The latter observation is based on symmetries of the Wronskian relation (4.1) and numerical computations which were carried out up to the Trotter number $N = 16$. To go beyond this bound requires more extensive numerical computations which are planned to be carried out in future work.

Another aspect which has been omitted from the present work is the derivation of integral equations similar to those non-linear integral equations which have been previously obtained on the basis of the Bethe ansatz equations; see e.g. [2] and references therein. The basis for such a derivation is numerical evidence for the distribution of the Bethe roots in the large Trotter number limit, $N \to \infty$. For this reason the discussion of integral equations and their connection with the thermodynamic Bethe ansatz are postponed until the necessary numerical data has been obtained.

For vanishing magnetic field the Wronskian relation ceases to be valid but in the text it was shown that at roots of unity one might be able to employ the same loop algebra symmetry as the one which exists for the six-vertex model. This might possibly help to reduce the order of equations or simplify the computation of the spectrum of the quantum transfer matrix.

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A. Properties of Q for generic q

For comparison with the line of argument for the classical six-vertex model the reader might wish to consult [8]. The line of argument closely follows the exposition given there.

A.1 The fusion hierarchy in terms of Q

Setting the free parameter s in ρ^+ to the special value $s = q^{2d},\ d = 1, 2, ...$ one derives the following identities by restricting the $\mathfrak{L}$ and $\mathfrak{L}^*$-operator given in (3.4) and (3.5) to the subspaces $V_{<d} = \text{span}\{|k\rangle\}_{k=0}^{d-1}$ and $V_{\geq d} = \text{span}\{|k\rangle\}_{k=d}^{\infty}$,

$$s = q^{2d} :\ \mathfrak{L}^*(z)|_{V_{<d}} = q^d(1 \otimes q^{\frac{d}{2}\sigma^z})L^{*(d-1)}(zq^d)(1 \otimes q^{-d\sigma^z}) \tag{A.1}$$

$$s = q^{2d} :\ \mathfrak{L}^*(z)|_{V_{\geq d}} = q^{2d}(1 \otimes q^{d\sigma^z})\mathfrak{L}^*(zq^{2d}; s \to q^{-2d})(1 \otimes q^{-2d\sigma^z}) \tag{A.2}$$

Employing that by construction the Q-operator commutes with the alternating spin-operator, $[Q, S_A] = 0$, one deduces from these last two equations the following identity for the higher spin quantum transfer matrices,

$$\tau^{(d-1)}(z) = q^{d(\alpha - S_A)}Q(zq^{-d}; s = q^{2d}) - q^{d(S_A - \alpha)}Q(zq^d; s = q^{-2d})\ . \tag{A.3}$$

Below we will see that this relation can be simplified further due to a factorisation of the Q-operator into two parts.

A.2 Algebraic Bethe ansatz computation

In order to obtain the eigenvalues we apply the algebraic Bethe ansatz for the quantum transfer matrix (see e.g. [3]) and compute the action of Q on a Bethe state. Denote by $\{\uparrow, \downarrow\}$ by the orthogonal basis in $\mathbb{C}^2$ and consider the reference state

$$|0\rangle = \downarrow \otimes \uparrow \cdots \otimes \downarrow \otimes \uparrow\ . \tag{A.4}$$

Let $\{A, B, C, D\}$ be the matrix elements of the quantum monodromy matrix (2.21) then a Bethe state is given by

$$\left| x_1^+, ..., x_{n_+}^+ \right\rangle := B(1/x_1^+) \cdots B(1/x_{n_+}^+) \left|0\right\rangle$$

with $\{x_1^+, ..., x_{n_+}^+\}$ being a solution to the Bethe ansatz equations (4.4). Since the auxiliary space of the quantum transfer matrix (1.2) and Q-operator (3.7) are the same as in the ordinary case of the classical six-vertex transfer matrix with quasi-periodic boundary conditions the results from [8] apply. Using the commutation relations between the matrix elements A, B, C, D and those of the monodromy matrix of the Q-operator,

$$\boldsymbol{Q}_{k,l}(z; s) := \langle k| \, q^{\alpha h_1 \otimes 1} \mathfrak{L}_N(zw)\mathfrak{L}^*_{N-1}(z/w) \cdots \mathfrak{L}_2(zw)\mathfrak{L}^*_1(z/w) \, |l\rangle\, , \tag{A.5}$$

detailed in [8] we obtain

$$Q(z; s) \left| x_1^+, ..., x_{n_+}^+ \right\rangle =$$

$$\left\{ \sum_{k=0}^{\infty} \langle 0| \, \boldsymbol{Q}_{kk}(z; s) \, |0\rangle \prod_{j=1}^{n_+} \frac{\langle k+1| \, \mathfrak{a}_j \, |k+1\rangle \, \langle k| \, \mathfrak{d}_j \, |k\rangle - \langle k| \, \mathfrak{c}_j \mathfrak{b}_j \, |k\rangle}{\langle k+1| \, \mathfrak{a}_j \, |k+1\rangle \, \langle k| \, \mathfrak{a}_j \, |k\rangle} \right\} \left| x_1^+, ..., x_{n_+}^+ \right\rangle$$

Here we have introduce the abbreviations

$$\mathfrak{L}(zx_j^+) = \begin{pmatrix} \mathfrak{a}_j & \mathfrak{b}_j \\ \mathfrak{c}_j & \mathfrak{d}_j \end{pmatrix} \tag{A.6}$$

for the matrix elements of the $\mathfrak{L}$-operator. Inserting the explicit expressions for the latter which can be read off from (3.4) one arrives at

$$\begin{aligned} Q(z;s)\left|x_1^+,...,x_{n_+}^+\right\rangle = \\ \left\{\sum_{k=0}^{\infty} \langle 0| \boldsymbol{Q}_{kk}(z;s)\,|0\rangle \prod_{j=1}^{n_+} \frac{q^{-2k-1}(1-z\;x_j^+)(1-zs\;x_j^+)}{(1-zsq^{-2k}\;x_j^+)(1-zsq^{-2k-2}\;x_j^+)}\right\} \;\left|x_1^+,...,x_{n_+}^+\right\rangle \\ = q^{S_A-\alpha}Q^+(z)Q^+(zs)\sum_{k=0}^{\infty}\frac{q^{2k(S_A-\alpha)}\mathcal{T}^{(0)}(zsq^{-2k-1})}{Q^+(zsq^{-2k})Q^+(zsq^{-2k-2})}\;\left|x_1^+,...,x_{n_+}^+\right\rangle\;. \end{aligned}$$

In the last line we have used the definition of Q^+ as a polynomial (3.14) and

$$\langle 0| \boldsymbol{Q}_{kk}(z;s)\,|0\rangle = q^{(n-\alpha)(2k+1)}[(zwsq^{-2k}-1)(zsq^{-2k-2}/w-1)]^n \;.$$

Taking the limit $s\to 0$ in order to fix the normalisation constant we deduce from this expression the following formula for Q^-,

$$Q^-(z) = Q^+(z)\sum_{k=0}^{\infty}\frac{q^{2k(S_A-\alpha)}\mathcal{T}^{(0)}(zq^{-2k-1})}{Q^+(zq^{-2k})Q^+(zq^{-2k-2})}\;. \tag{A.7}$$

Note that in [8] the vanishing of the unwanted terms in the Bethe ansatz has only been verified for $n_+ = 1,2,3$, since the algebraic Bethe ansatz computation is more involved than in the case of the transfer matrix due to the infinite-dimensional auxiliary space of the Q-operator. However, the result for the spectrum coincides with the one found at roots of unity and the eigenvalues satisfy all aforementioned functional relations for the Q-operator, which have been derived by different means. We shall take this as sufficient evidence that the algebraic Bethe ansatz computation presented above holds also true for $n_+ > 3$.

B. Properties of Q when q is a root of unity

Let us now turn to the case when q is a primitive root of unity of order ℓ.

B.1 Functional relations for the fusion hierarchy

The evaluation module ρ^+ is now finite-dimensional according to (3.3). For analysing the spectrum of Q we now rely on a functional relation derived in [9]. To connect with the discussion therein we set $r=\mu^{-1}$ and $s=\mu^{-2}$ in (3.1) and obtain the evaluation representation π_z^μ specified in equation (15-16) of [9]. Thus, in the following we refer to $\rho^+(r=\mu^{-1},s=\mu^{-2})$ as π_z^μ. Then the following short exact sequence holds (see equations (52-53) in [9]),

$$0\to\pi_{\mu q}^{\mu\nu q}\to\pi_{\mu\nu q^2}^{\mu}\otimes\pi_1^{\nu}\to\pi_{\mu q^{-\ell'+1}}^{\mu\nu q^{-\ell'+1}}\otimes\pi_{\nu q^{\ell'+1}}^{(\ell'-2)}\to 0\;. \tag{B.1}$$

Here $\pi_z^{(\ell'-2)}$ is the evaluation representation of spin $(\ell'-1)/2$. As before this decomposition of the tensor product of representations implies a functional relation, but this time it involves a product of two Q-operators with different values for the free parameters entering (3.1). Setting $s=\mu^{-2}$ and $t=\nu^{-2}$ this functional relation reads

$$Q(zq^2/s;s)Q(z;t)=q^{S_A-\alpha}Q(zq^2/s;stq^{-2})[(zq^2-1)^n(z-1)^n+q^{\ell'(S_A-\alpha)}\tau^{(\ell'-2)}(zq^{\ell'+1})]\ , \tag{B.2}$$

compare with equation (46) in [10]. Assume that $[Q(z_1;s_1),Q(z_2;s_2)]=0$ for arbitrary pairs $z_{1,2},s_{1,2}\in\mathbb{C}$. This has been proved for $\ell=3,4,6$ by explicitly constructing the corresponding intertwiner for $\rho^+(z_1,s_1)\otimes\rho^+(z_2;s_2)$ [16, 17]. Thus, the eigenvalues of $Q(z;s)$ must be polynomial in z (and s) their most general form being

$$Q(z;s)=\frac{1-q^{2\ell'(S_A-\alpha)}}{q^{\alpha-S_A}-q^{S_A-\alpha}}\prod_{j=1}^{k}(1-z\ x_j)\prod_{j=1}^{N-k}(1-z\ y_j(s))\ .$$

Here we have taken the limit $z\to 0$ to fix the normalisation constant,

$$\lim_{z\to 0}Q(z;s)=\operatorname*{Tr}_{\rho^+}q^{(\alpha-S_A)h_1}\ . \tag{B.3}$$

We assume that the roots $x_j=x_j^+$ are independent of s while the y_j's depend on it allowing for the possibilities that either $k=0$ or $k=N$. Inserting this general expression for the eigenvalue into (B.2) one deduces that the roots $y_j(s)$ can only depend linearly on s, i.e. $y_j(s)=x_j^-s$ for some x_j^-. This implies the factorisation (3.9) in the text. Futhermore we infer from (3.12) that $k=N/2-S_A$ in each fixed S_A sector.